Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

A coarse-grained molecular model of graphene: application to graphene-based multilayered nanocomposites

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ABSTRACT

Single-layer graphene exhibits remarkable electronic and thermal properties and it is the strongest material known, thus it offers great promise for a broad range of nanotechnological applications. Despite the exceptional properties exhibited by pristine graphene monolayers, harnessing the mechanical performance of single-sheets at larger length scales or for higher material hierarchies (e.g., graphene paper) remains a bottleneck. One promising strategy is to enhance the interlayer shear strength by addition of a soft material phase such as polymer or proteins. However, and despite extensive experimental efforts, the physical mechanisms that govern the mechanical performance of this new generation of graphene-based composite materials remain poorly understood. In order to obtain a comprehensive physical understanding of the behavior of graphene-based nanocomposites that would lead to rational design of these materials, a multiscale approach is required. Coarse-grained models, where groups of atoms are clustered in beads that interact through an effective potential, offer great promise as they allow simulating mesoscale physical processes while retaining the molecular detail of the system. Current coarse-grain models of graphene suffer from some critical shortcomings that prevent them from being applicable to the study of graphene-based nanocomposites, namely, they have not been optimized to accurately capture the mechanical properties of covalently bonded carbon-based materials, they are unable to capture the interlayer shear landscape between graphene sheets, and none of the existing approaches allows fracture of covalent bonds, which results in unrealistic behavior when the system is subjected to large deformations. Here, we present a novel coarse grain model of graphene that enables simulating large deformation and failure of large scale graphene-based hierarchical systems with a ~1000 fold increase in speed with respect to reactive force fields necessary to capture equivalent physical processes. Similarly to the Martini approach, the proposed model is compatible with existing coarse grain representations of proteins or polymers. The hexagonal symmetry of the graphene lattice is conserved in the coarse grain model, allowing it to capture the anisotropic mechanical behavior in the zigzag and armchair directions and possible asymmetries in the adsorption mechanisms of macromolecules. The force-field parameters of the model are calibrated using conservation of strain energy between the atomistic or continuum representations and the reduced order model. The bonded interactions in the model are anharmonic and can break, which allows capturing the nonlinear response and failure of graphene. Ultimately, the model captures the interlayer shear rigidity and the physical phenomena known as superlubricity.